Fall 2020

CHEM 725-138: Independent Study I

Farnaz Shakib

CEHM 725-138, Independent Study I - Fall 2020

Instructor: Farnaz A. Shakib, Ph.D.

Office: Tiernan 368
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Office Hours: M, W 10:00 am – 11:00 am. And by appointment.

Textbook: There is no textbook for this course. Lecture notes will be provided for the students.

Course Content: Tentative material to be covered.

Discussion 1. Introduction to Molecular Dynamics
Discussion 2. Concepts of Phase-Space and Hamiltonians
Discussion 3. Born-Oppenheimer Approximation and Potential Energy Surfaces
Discussion 4. Force Fields
Discussion 5. Solving the Equations of Motion
Discussion 6. Constraints in Molecular Dynamics
Discussion 7. Constant Temperature/Pressure Simulations
Discussion 8. Monte Carlo Simulations
Discussion 9. Time-Correlation Functions
Discussion 10. Mixed Quantum-Classical Dynamics
Discussion 11. Surface-Hopping Dynamics

Learning outcomes

After successful completion of the course students will

- understand the theoretical principles of MD simulations
- know typical application areas, and can assess the suitability of a method to a given problem
- can independently design a simulation for a relatively simple scientific problem
- understand the significance of basic algorithms and their parameters for a successful simulation
- understand the method well enough to be able to carry out research in this area independently

Final Evaluation

Students will make a presentation on a recently published paper which uses MD techniques in chemistry, biochemistry or materials science.

Grading

Choice of Appropriate References Material: 20%
Quality of Presentation Slides: 30%
Final Presentation: 50%
A (90-100%), B+ (85-89.9%), B (80-84.9%), C+ (75-79.9%), C (70-74.9%), D (60-69.9%), F(<60%)